

Octaneperoxoic acid
33734-57-5 | DTXSID7074618

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.45

Global applicability domain: Inside

Local applicability domain index: 3.98e-01

Confidence level: 5.29e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Molinate

Measured: 25.7

Predicted: 14.8

[Image not found](#)

Acetamide, N-methyl-N-phenyl-

Measured: 1.51

Predicted: 2.53

[Image not found](#)

Butyl ether

Measured: 72.4

Predicted: 32.3

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Azacyclotridecan-2-one

Measured: 2.57

Predicted: 4.16